

# Delocalization transitions of semi-flexible manifolds

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Semi-flexible manifolds such as fluid membranes or semi-flexible polymers undergo delocalization transitions if they are subject to attractive interactions. We study manifolds with short-ranged interactions by field-theoretic methods based on the operator product expansion of local interaction fields. We apply this approach to manifolds in a random potential. Randomness is always relevant for fluid membranes, while for semi-flexible polymers there is a first order transition to the strong coupling regime at a finite temperature.

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Low dimensional manifolds play an important role in a variety of different contexts, e.g., as soft matter objects or as domain boundaries in condensed matter systems. They can perform large shape fluctuations driven by entropy [1]. According to their fluctuations they can be divided into two classes. *Flexible* manifolds, such as interfaces, polymerized membranes, and long polymers, fluctuate under a *tension* controlling their area or length. The other class is governed by *bending energy*; i.e., regions of high *curvature* are penalized. Examples are polymers not much longer than their persistence length, like actin or DNA, and fluid membranes. These objects are stiffer, and we call them *semi-flexible* manifolds.

Whenever a fluctuating manifold is attracted towards some other “defect” manifold, there is a competition between freely fluctuating configurations favored by entropy and configurations bound to the defect, which are preferred by energy. This competition can lead to a phase transition, the so called delocalization or unbinding transition. It is often of second order, that is, the amplitude of the fluctuations diverges continuously as the transition point is approached from within the bound phase. This leads to a scaling regime close to the transition whose universal characteristics can be described by a continuum field theory. Well-known examples of delocalization are wetting phenomena [2]. For interfaces and polymers, these transitions have been widely studied [3]. In the case of polymers, even the generalized problem of  $N$  mutually attracting objects can be treated. Analytically continued to  $N = 0$ , this describes a directed polymer in a random medium [4], which in turn is related to theories of stochastic surface growth [5]. The delocalization transition then corresponds to a roughening transition between a smooth and a rough growth mode.

An important class of low-dimensional manifolds are stretched objects with mainly transversal fluctuations. These are described by a  $d$ -dimensional displacement field  $\mathbf{r}(t)$  which depends on a  $D$ -dimensional internal variable  $t$ . The continuum Hamiltonian takes the form

$$\mathcal{H} = \int \left[ \frac{1}{2} (\nabla^k \mathbf{r})^2 + V(\mathbf{r}, \nabla \mathbf{r}) \right] d^D t, \quad (1)$$

where  $(\nabla^k \mathbf{r})^2 \equiv \sum_{\alpha=1}^D \sum_{i=1}^d (\partial^k r_i(t) / \partial t_{\alpha}^k)^2$  is the leading tension ( $k = 1$ ) or curvature ( $k = 2$ ) energy in a small-gradient expansion. The potential  $V$  describes the interaction of the manifold with an external object or boundary at  $\mathbf{r} = 0$ , or the mutual interaction between two manifolds with relative displacement  $\mathbf{r}(t)$ . Physical realizations of flexible manifolds ( $k = 1$ ) are directed polymers and flux lines in a type II superconductor ( $D = 1, d = 2$ ) [6,7], steps on a tilted crystal surface ( $D = 1, d = 1$ ), and domain walls in a ferromagnet ( $D = 2, d = 1$ ). Short-ranged interactions of definite sign can be represented as  $V(\mathbf{r}(t)) = g\Phi(t)$  in terms of the local *contact field*

$$\Phi(t) \equiv \delta(\mathbf{r}(t)). \quad (2)$$

The scaling dimension of this field,  $x_{\Phi} = d\chi$ , is given in terms of the roughness exponent  $\chi$ , with  $\chi = (2 - D)/2$  for  $k = 1$ . There exists a well known perturbative framework [8,9] to treat such interactions, which has been applied extensively to the problem of self-avoiding manifolds [10–14]. More complicated short-ranged [15] and long-ranged [16] interactions have been studied as well.

In this Letter, we develop the field theory of semi-flexible manifolds with local interactions, described by the Hamiltonian (1) with  $k = 2$ . Physically interesting cases are again polymers ( $D = 1, d = 1, 2$ ) [17–19] and, in particular, fluid membranes ( $D = 2, d = 1$ ) [20]. Since a semi-flexible manifold has a locally well-defined orientation, we have to consider interactions  $V(\mathbf{r}(t), \nabla \mathbf{r}(t))$  that depend both on the displacement and on the orientation. We find there are now two important scaling fields: Local contacts at arbitrary orientation are still represented by the field  $\Phi(t)$  given by (2), which has dimension  $x_{\Phi} = d\chi$  with  $\chi = (4 - D)/2$ . Due to the stiffness, however, closeby contacts always have a preferred orientation parallel to the defect. Such contacts are described by the field

$$\Omega(t) \equiv \delta(\mathbf{r}(t))\delta(\nabla \mathbf{r}(t)) \quad (3)$$

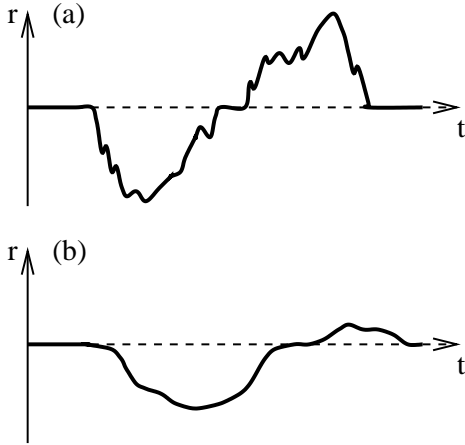


FIG. 1. (a) A flexible and (b) a semiflexible polymer  $r(t)$  bound to an attractive defect indicated by the dashed lines. The unbound segments join the defect at arbitrary orientation and at fixed orientation  $dr/dt = 0$ , respectively.

of dimension  $x_\Omega = d\chi + dD(\chi - 1)$ . The scaling fields  $\Phi$  and  $\Omega$  are found to obey an operator product expansion. This is a well-known concept in field theory (see, e.g., Ref. [21]), which has been applied extensively to flexible manifolds [22]. It allows us to write down renormalization group equations for generic local interactions. This leads to results for the delocalization of semi-flexible polymers and of fluid membranes. Most importantly, the bound state of a semi-flexible manifold turns out to be maintained by contact interactions (3) at fixed orientation, while the bound state of a flexible manifold involves interactions of the form (2). Typical bound state configurations are compared in Fig. 1 for the case of polymers ( $D = 1$ ). Our one-loop results are in agreement with previous results obtained by approximate renormalization methods [23,24] and by approaches specific to polymers [17–19]. They are exact for  $D = 1$  and can be improved systematically for higher values of  $D$ . Furthermore, they can be applied to a semi-flexible manifold in a quenched random potential (taken to be Gauss distributed with mean  $\overline{V(\mathbf{r}, t)} = 0$  and variance  $\overline{V(\mathbf{r}, t)V(\mathbf{r}', t')} = \sigma^2\delta(t - t')\delta(\mathbf{r} - \mathbf{r}')$ ). In the replica formalism, this is equivalent to  $N$  interacting semi-flexible manifolds in the limit of vanishing  $N$ . For fluid membranes, any amount of disorder is relevant and leads to a strong coupling phase. For semi-flexible polymers, however, small amounts of disorder are irrelevant (unlike for their flexible counterparts). There is now a first-order transition to the strong coupling phase at a finite amount of disorder. A quantitative description of the disordered strong coupling phase is, however, beyond the means of perturbation theory.

We study the manifold displacement field in a hypercube of longitudinal extension  $0 \leq t_\alpha \leq T$  ( $\alpha = 1, \dots, D$ ) and of transversal extension  $0 \leq r_i \leq R$  ( $i = 1, \dots, d$ ). For  $T \gg R^{1/\chi}$ , the free energy becomes extensive,  $F \sim T^D R^{-D/\chi}$ , and the perturbation series for the free en-

ergy density  $f \equiv F/T^D$  becomes invariant under translations of  $t$ . This series takes the easiest form if the manifold is subject to *wall constraints* forcing the probability density  $\rho(\mathbf{r}') \equiv \langle \delta(\mathbf{r}(t) - \mathbf{r}') \rangle$  to vanish on the boundary of the hypercube, in particular along the “edge”  $\mathbf{r} = 0$ . The density then takes the asymptotic scaling form  $\rho(\mathbf{r}) \sim (r_1 \dots r_d)^\theta R^{-d(1+\theta)}$  for  $|\mathbf{r}| \ll R$ , with an exponent  $\theta > 0$  expressing long-ranged suppression of the configurations close to the boundary. The wall constraint is natural in  $d = 1$  for a fluid membrane at a planar system boundary, or for a pair of membranes without mutual intersections. The generalization to arbitrary  $d$  has been chosen such that the Hamiltonian (1) remains factorizable. Short-ranged interactions with the manifold  $\mathbf{r} = 0$  are now described by the local field

$$\Omega(t) \equiv \lim_{r \rightarrow 0} r^{-d\theta} \prod_{i=1}^d \delta(r_i(t) - r), \quad (4)$$

whose expectation values are finite. Due to the constraint, these interactions are always at fixed orientation  $\nabla \mathbf{r} = 0$ . Hence, we have used the same symbol  $\Omega$  as for the field (3) of the unconstrained system. The correlation functions

$$\langle \Omega(t) \rangle \sim R^{-x_\Omega/\chi} \quad (5)$$

$$\langle \Omega(t)\Omega(t') \rangle \sim |t - t'|^{-x_\Omega} \langle \Omega(t) \rangle + \dots \quad (|t - t'| \ll R) \quad (6)$$

define the scaling dimension  $x_\Omega$ . In the constrained system, the density (5) is linked to the pressure of the system by a wall theorem,

$$\langle \Omega \rangle \sim (\partial f / \partial R)^d \sim R^{-d(1+D/\chi)}. \quad (7)$$

This determines the exponent value [25]

$$x_\Omega = d(\chi + D), \quad (8)$$

which differs from that of the unconstrained system. It is in agreement with a conjecture from functional renormalization [26] for general  $D$  and a direct calculation [27] for  $D = 1$ .

The interaction part  $\delta f(h, R) \equiv f(h, R) - f(0, R)$  of the free energy of the system with  $V(\mathbf{r}(t), \nabla \mathbf{r}(t)) = h\Omega(t)$  can be expanded as a power series

$$\delta f = h\langle \Omega \rangle + \frac{h^2}{2} \int d^D t \langle \Omega(0)\Omega(t) \rangle_c + O(h^3) \quad (9)$$

containing the connected correlation functions

$$\langle \Omega(0)\Omega(t) \rangle_c \equiv \langle \Omega(0)\Omega(t) \rangle - \langle \Omega \rangle^2 \quad (10)$$

etc., taken at  $h = 0$ . By (8), there is a whole *line* in the  $(D, d)$  plane, where the interaction  $\Omega$  is marginal, i.e., where  $x_\Omega = D$ . This line is given by

$$d^*(D) = \frac{2D}{4 + D}. \quad (11)$$

The perturbation series (9) has poles in

$$\epsilon \equiv D - x_\Omega = D - d(2 + D/2), \quad (12)$$

which can be regularized around *any point* on the line of marginality (11); see the discussion in [10] for flexible manifolds. The singularity of the two-point function (10) is given by the operator product expansion

$$\Omega(t)\Omega(t') \sim |t - t'|^{-x_\Omega}\Omega(t) + \dots \quad (13)$$

This singularity determines in a standard way [22] the one-loop renormalization group equation of the dimensionless coupling constant  $v \equiv hR^{\epsilon/\chi}$ . In an appropriate scheme, this takes the form

$$\dot{v} = \epsilon v - v^2 + O(v^3). \quad (14)$$

The unstable fixed point  $v^* = \epsilon + O(\epsilon^2)$  represents the transition. The linearized form  $\dot{v} = \epsilon^*(v - v^*) + \dots$  with  $\epsilon^* = -\epsilon + O(\epsilon^2)$  then determines the scaling of the transversal localization length  $\xi \equiv \langle \mathbf{r}^2 \rangle^{1/2}$ ,

$$\xi \sim (v^* - v)^{-\chi/\epsilon^*} \quad (v < v^*), \quad (15)$$

and the scaling dimension

$$x_\Omega^* = D - \epsilon^* = 2D - x_\Omega + O(\epsilon^2), \quad (16)$$

which takes the place of  $x_\Omega$  in the correlations (5) and (6) at the transition point. These relations describe the scaling of a bound state maintained by contact forces at fixed orientation. Typical configurations look similar to those of Fig. 1(b) but are confined to the region  $r_i > 0$ .

The most interesting application of (15) and (16) is the delocalization transition of a fluid membrane from a hard wall ( $D = 2, d = 1$ ), where  $\xi \sim (T_c - T)^{-1}$  (since the effective coupling is temperature-dependent) and  $x_\Omega^* = 1$ . Not surprisingly, these one-loop results are in agreement with those from functional renormalization [23]. They also fit very well the numerical values of [24], which implies that higher order corrections must be small. The system with wall constraint at  $h = 0$  can be regarded as an unconstrained system in the limit of large repulsive interaction. Conversely, the scaling at the transition point of the constrained system may be related to that of the free unconstrained system. Indeed, the one-loop value  $x_\Omega^*$  from (16) equals the dimension  $x_\Omega = 1$  of the free field (3), indicating that the sum of the higher order corrections in (14) and (16) may vanish altogether at the specific point ( $D = 2, d = 1$ ).

For the case of polymers ( $D = 1$ ) it is easy to show that the multi-point correlations entering (9) factorize after “time-ordering” the interaction points,

$$\langle \Omega(t_1) \dots \Omega(t_n) \rangle = \langle \Omega(t_1) \rangle \mathcal{R}(t_2 - t_1) \dots \mathcal{R}(t_n - t_{n-1}) \quad (17)$$

for  $t_1 < \dots < t_n$ . The factors  $\mathcal{R}(t) \equiv \langle \Omega(0)\Omega(t) \rangle / \langle \Omega \rangle$  can be interpreted as “return” probabilities. Using (17), one can show that the polymer perturbation series (9) is *one-loop renormalizable*; i.e., the connected two-point function  $\langle \Omega(0)\Omega(t) \rangle_c$  generates the only primitive singularity, and there are no higher-order terms in (14). The arguments are completely analogous to those for the case  $k = 1$  [8,22]. The implications of (15) and (16) on general semi-flexible polymers are discussed and verified numerically in [28]. Here we have given a *unified derivation* of these relations, stressing the theoretical analogies with their known counterparts for  $k = 1$  [29,22].

We now turn to systems without the wall constraint and restrict ourselves to  $D = 1$ , namely mutually interacting semiflexible polymers and, in particular, a single such polymer in a random medium. The latter system has a possible biostatistical application in the theory of sequence alignment [30]. In the absence of a wall constraint, we have to study generic contact interactions  $V(t) = g\Phi(t) + h\Omega(t)$  involving the fields (2) and (3). The perturbation series then contains connected correlations  $\langle \Phi(t_1) \dots \Phi(t_n)\Omega(t'_1) \dots \Omega(t'_m) \rangle$  in the free theory ( $g = h = 0$ ), which can be computed exactly. They can be shown to obey the operator product expansion

$$\Phi(t)\Phi(t') \sim |t - t'|^{-d}\Omega(t) + \dots \quad (18)$$

$$\Phi(t)\Omega(t') \sim |t - t'|^{-\frac{3}{2}d}\Omega(t) + \dots \quad (19)$$

$$\Omega(t)\Omega(t') \sim |t - t'|^{-2d}\Omega(t) + \dots \quad (20)$$

These relations just say that *any* pair of closeby contacts amounts to a single contact at fixed orientation, multiplied by a singular prefactor. These singularities determine the one-loop renormalization group equations

$$\dot{u} = (1 - 3d/2)u \quad (21)$$

$$\dot{v} = \epsilon v - v^2 - u^2 - cuv \quad (22)$$

for the dimensionless couplings  $u \equiv gR^{(1-3d/2)/\chi}$  and  $v \equiv hR^{\epsilon/\chi}$  with

$$\epsilon \equiv 1 - x_\Omega = 1 - 2d. \quad (23)$$

The corresponding flow diagram for  $d = 1$  is shown in Fig. 2. The unique delocalization fixed point ( $u^* = 0, v^* = \epsilon$ ) is on the line  $u = 0$ . This property ensures that the constant  $c$  in (22) drops out of the critical exponents. It will be preserved for any  $d > 2/3$  also at higher orders since any operator product  $\prod_{i,j} \Phi(t_i)\Omega(t'_j)$  couples only to  $\Omega(t_1)$ . The perturbation series at  $u = 0$ , however, is factorizable according to (17) and one-loop renormalizable in exactly the same way as with the wall constraint. Hence, the (in  $D = 1$ ) exact relations (15) and (16) still hold (with  $\epsilon$  given by (23) and  $x_\Omega = 2d$ ), resulting in  $\xi \sim (T_c - T)^{3/(2-4d)}$  for  $2/3 < d < 1$  and  $x_\Omega^* = 2 - 2d$ . This scaling dimension turning negative for  $d > 1$  indicates that the transition becomes of first order; see the discussion and extensive numerics in [28]. An analogous first-order regime is known for flexible polymers [29].

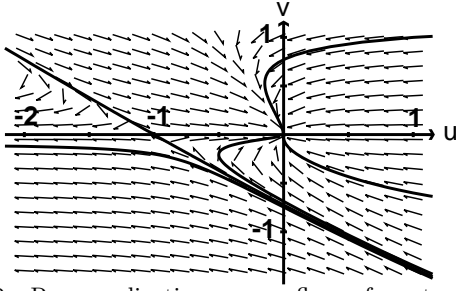


FIG. 2. Renormalization group flow of contact interactions for a semi-flexible polymer in  $1 + 1$  dimensions. The flow equations (21), (22) have the single unstable fixed point  $(u, v) = (-1, 0)$  marking the delocalization transition.

The above arguments can be generalized to the replica theory of  $N$  semiflexible polymers coupled by pair contact forces. If these are of type  $\Omega$ , the time-ordered perturbation series can be mapped term by term onto the perturbation series of flexible polymers with  $\Phi$  interactions. Its leading divergencies are due to “ladder” diagrams with the same pair of polymers interacting at subsequent points  $t_i$  [31,32]. The presence of  $\Phi$  interactions for semiflexible polymers does not change these singularities by the same argument as for  $N = 2$ : Due to their stiffness, any two semi-flexible polymers interacting twice in a short interval have to be parallel to each other, or, in other words, the leading divergent diagrams behave like diagrams involving only  $\Omega$  operators. For the  $\Omega$  system, however, the results of [31,32] immediately carry over and imply that the critical behavior at the delocalization transition does not depend on  $N$ . In particular, the random limit of vanishing  $N$  becomes trivial. We conclude that a  $1 + d$  dimensional semi-flexible polymer in a random potential has a phase transition between a weak and a strong coupling phase at a critical strength of the randomness for  $d > 2/3$ . This phase transition corresponds to the roughening transition of the Kardar-Parisi-Zhang equation in  $4d$  dimensions. For fluid membranes, on the other hand, an arbitrarily small amount of disorder is relevant and leads to a strong coupling phase.

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[1] For a review, see R. Lipowsky, *Physica Scripta* **T29**, 259 (1989).

- [2] For a review, see M.E. Fisher, *J. Chem. Soc. Faraday Trans. 2* **82**, 1569 (1986).
- [3] G. Forgacs, R. Lipowsky, and Th.M. Nieuwenhuizen, in *Phase Transitions and Critical Phenomena*, Vol. 14, (Academic Press, London, 1991), and references therein.
- [4] M. Kardar, *Phys. Rev. Lett.* **55**, 2235 (1985); *Nucl. Phys. B* **290**, 582 (1987).
- [5] M. Kardar, G. Parisi, and Y.-C. Zhang, *Phys. Rev. Lett.* **56**, 889 (1986).
- [6] G. Blatter, M.V. Feigel'man, V.B. Geshkenbein, A.I. Larkin, and V.M. Vinokur, *Physica A* **200**, 341 (1993).
- [7] L. Balents and M. Kardar, *Phys. Rev. B* **49**, 13030 (1994).
- [8] B. Duplantier, *Phys. Rev. Lett.* **62**, 2337 (1989).
- [9] F. David, B. Duplantier, and E. Guitter, *Phys. Rev. Lett.* **70**, 2205 (1993); *Nucl. Phys. B* **394**, 555 (1993).
- [10] M. Kardar and D.R. Nelson, *Phys. Rev. Lett.* **58**, 1289 (1987).
- [11] T. Hwa, *Phys. Rev. A* **41**, 1751 (1990).
- [12] B. Duplantier, T. Hwa, and M. Kardar, *Phys. Rev. Lett.* **64**, 2022 (1990).
- [13] F. David, B. Duplantier, and E. Guitter, *Phys. Rev. Lett.* **72**, 311 (1994).
- [14] F. David and K.J. Wiese, *Phys. Rev. Lett.* **76**, 4564 (1996); *Nucl. Phys. B* **487**, 529 (1997).
- [15] M. Lässig and R. Lipowsky, *Phys. Rev. Lett.* **70**, 1131 (1993).
- [16] M. Lässig, *Phys. Rev. Lett.* **77**, 526, 1996.
- [17] A.C. Maggs, D.A. Huse, and S. Leibler, *Europhys. Lett.* **8**, 615 (1989).
- [18] R. Lipowsky, *Phys. Rev. Lett.* **62**, 704 (1989).
- [19] G. Gompper and T.W. Burkhardt, *Phys. Rev. A* **40**, 6124 (1989).
- [20] R. Lipowsky, in: R. Lipowsky, E. Sackmann (eds.), *Structure and Dynamics of Membranes, Handbook of Biological Physics* **1**, Elsevier, Amsterdam, 521 (1995).
- [21] J. Cardy, *Scaling and Renormalization in Statistical Physics* (Cambridge University Press, Cambridge, 1996).
- [22] For a review, see M. Lässig, *J. Phys. C* **10**, 9905 (1998).
- [23] R. Lipowsky, *Europhys. Lett.* **7**, 255 (1988).
- [24] R. Lipowsky and B. Zielinska, *Phys. Rev. Lett.* **62**, 1572 (1989).
- [25] G. Gompper, private communication; G. Gompper and D. Kroll, *J. Phys I France* **1**, 1411 (1991).
- [26] R. Lipowsky, *Z. Phys. B* **97**, 193 (1995).
- [27] T.W. Burkhardt, *J. Phys. A* **26**, L1157 (1993).
- [28] R. Bundschuh, M. Lässig, and R. Lipowsky, preprint (1999).
- [29] R. Lipowsky, *Europhys. Lett.* **15**, 703 (1991).
- [30] T. Hwa and M. Lässig, *Phys. Rev. Lett.* **76**, 2591 (1996).
- [31] M. Lässig, *Nucl. Phys. B* **448**, 559 (1995).
- [32] R. Bundschuh and M. Lässig, *Phys. Rev. E* **54**, 304 (1996).